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ABSTRACT

A university level course which uses minicomputers in laboratory data acquisition and experimental control is described. The majority of the students are chemistry seniors and graduate students; prerequisites are general physics and one semester of computer science or programing experience. The goals of the course, which is divided into 3 5-week parts, are to develop a systematic technique for data acquisition and control of an analytical instrument using a digital computer. The first part of the course deals with the electronics involved in interfacing; the second part concentrates on programing the computer to do an analysis of the data and the assembler language subroutines; the third part is devoted to individual student projects. The majority of the programing is done in BASIC which was chosen for its ease in learning, its immediate debugging capabilities and its comparability with previous teaching experience. A list of projects performed by students at Texas Christian University during the past two years is included, as is a course schedule. (Author/KKC)

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Laboratory Automation for Physical Scientists

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During the past few years several papers have been presented at these conferences describing the use of minicomputers in laboratory data acquisition and experimental control. Much of what has been developed here at TCU has been influenced by the results (both positive and negative) of these authors.

One of the initial decisions to be made was whether to include computerization in the existing analytical chemistry or physical chemistry courses or to provide a separate three hour elective course. The latter option was taken to prevent dilution of basic concepts from the existing chemistry courses. Although the primary source of students has been chemistry seniors and graduate students, students from all of the physical sciences have been invited to be in the course. A separation of students by major curriculum is in Table II.

Another choice was that of a programming language to be used. BASIC was chosen for 1) ease in learning, 2) immediate debugging and 3) compatability with previous teaching experience. The design of the course is of course partly dictated by the computer and interfacing equipment available and the background of the students enrolled in the course.

At TCU we have about five research projects interfaced to a PDP-11/20 minicomputer. This computer is "time-shared", on a per hour time slice, between students and researchers. The I/O devices available include an ASR-33 teletype, high speed paper tape reader, magnetic tape, and three digital I/O interfaces (DR-11-A), one of which is reserved for student use. The interface between instrument and computer is constructed using Heath digital-analog logic modules (Malmstadt & Enke, designed). These modules allow off-line connections to be made and tested to some extent before

connecting to the computer via the DR-11. The similar TTL levels eliminate any level conversion problems and assures some degree of safety to computer during the connection.

The prerequisites of the course are general physics and one semester of computer science or programming experience. Usually the experience is in batch FORTRAN but a few students have had some assembler language experience. For these few I try to assign problems which involve more assembler programming than for the majority of the class. Although a year of physics is a prerequisite, most of the students need as much review of basic dc electricity as possible.

The goals of the course are to develop a systematic technique for data acquisition and control of an analytical instrument using a digital computer. At almost every lecture session an attempt is made to place the current topic in its proper perspective in the total plan so that the goal is kept in sight.

In general, the course is divided into 3 5-week parts. A schedule is outlined in Table I. The first part deals with the electronics involved in interfacing. In particular, the various devices such as operational amplifiers, D/A and A/D converters, comparators, logic gates, and clocks are discussed in some detail, with the laboratory sessions using Heath digital logic modules off-line from the computer. Classroom demonstrations are used as an introduction to the use of the logic modules with the laboratory sessions remaining open at the convenience of the student. A class of 11 students using only two logic modules requires a do-it-yourself approach to the laboratory sessions. For senior students this works reasonably well. Encoders, decoders, stepper motors, asychronous motors, servo mechanisms and sensing devices are introduced during the last 5-week period since they

are not available for laboratory demonstration (at the present time) but are obviously important components in most control systems.

The second part concentrates on programming the computer to do an analysis of the data and the assembler language subroutines involved in handling interrupts, reading A/D converters and general digital I/O features. The majority of the programming is done in BASIC using the single user BASIC as supplied with the PDP-11 paper tape software. One modification was made to BASIC (as supplied from DEC) to allow the use of interrupts from an internal 60 cycle clock and from external sources thru the digital I/O interface (DR-11-A). Subroutine calls are made from BASIC using the EXF (n, A, B) function where the argument n is the pointer to the proper subroutine. Values of n may range from 0 to 19 as the system is presently configured. The remaining arguments, A and B, if needed, are evaluated in the assembler routine. The one restriction on the use of this EXF is that BASIC treats it as a function, i.e. only one value may be returned to BASIC from the assembler subroutine. For those problems requiring more than one value be returned, some programming tricks may be applied using the internal GETADR routine for an array and then putting values directly into the BASIC array. Several EXF functions have been written by the author to read or write records to magnetic tape and paper tape. These are available to all students for a more permanent storage of data for later analysis, in those cases where immediate analysis is not possible.

The last 5-week period is devoted to individual student projects, with class time reduced to 2 sessions per week. During the class periods, discussions are held involving problems with multiple variables, requiring

interaction logic and priority scheduling. These are not included as laboratory projects but are discussed so that students get some feeling for the relation between simple single variable problems and those of more complexity. As mentioned earlier, other electronic sensing devices, multiplexing, servo motors, etc. are discussed during this period. Also during this period each student is applying the knowledge and techniques developed during the first 10 weeks toward a special interfacing project involving one analytical instrument, usually of his choice.

Something needs to be mentioned with regard to the operation of the laboratory for this course. With one computer, one interface and two Heath logic modules available, it was necessary to make the laboratory session operate on an arranged basis rather than all together. A schedule sheet is available for advanced reservation of the equipment (by both researchers and students) and following each session the student must return the equipment to its normal state. This situation is somewhat difficult for both student and instructor in that little or no supervision is possible during most of the laboratory periods. Fortunately most students are seniors or graduate students with some past experience on individual projects and the situation has worked moderately well. The existing conditions require the student to dismantle his interface after each session to allow the next user to use the equipment. This forces the interface to be relatively simple but on the bright side requires students to document their wiring well at the close of each session so that at their next session the interfaces may be constructed rapidly to the point of the latest documentation. The value of documentation is thereby reenforced in each student's mind. This also demonstrates the value of the easy wiring aspect of the Heath modules.

A list of instruments and projects performed by students during past two years is given in Table III. The analytical instruments used in these projects are borrowed from some chemistry laboratory and returned at the end of the interfacing project. Little or no changes are made to the instruments themselves and often the student has previously used this particular instrument as an analytical tool so that the experimental set-up and data analysis are familiar to him and only the interface and programming need to be learned.

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Table 1. Course Schedule

Week		Topic
1	Electronics	Introduction to course; dc circuits; transistors;diodes;
2		Logic gates; timing conditions; logic levels; counters; clocks
3		Operational amplifiers
4		Comparator circuits; D/A converters
5		A/D converters; TEST on electronics
6	Programming	BASIC programming; standard deviations
7		linear least squares; non-linear least squares
8		PDP-11 Assembler language programming,
9		Emphasis on subroutine linkage to BASIC and data acquisition I/O routines, interrupt handling, A/D converter logic
10		Proposal of term project; data acquisition project from pH meter using op amp and A/D converter.
11-12	Individual Projects	Class periods reduced to twice per week In class discussions of stepper motors, shaft encoders, servo mechanisms, sensing devices, etc. which are not demonstrable in the laboratory
13-14		Large problems invlving multiple variables interactions and priority scheduling. During this time the student is working on his term project with an analytical instrument and doing the programming.
15		Oral reports in class on term projects.
16		Written reports due. Review. Final Exam.

Table II. Enrollment by major curriculum

	Spring 1973	Spring 1974
chemistry	11	5
psychology	1	2
computer science	1	1
physics		2
biology		1

Table III. Typical Student projects

Titration using pH meter
Polarograph
Gas chromatograph
Joyce-Loebl Microdensitometer - Sedimentation Velocity
Joyce-Loebl Microdensitometer - Molecular Weight
Photo digitalization
Physiological nerve impulse recording
Reaction calorimetry
Computer generated music
Photometer
Display of single valued function (vs. time) on standard oscilloscope.
Monitoring temperature & salinity of aquarium.